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An Integrated Chemical-Thermal-Mechanical-Hydrocode for Predicting the Response of AP/Al/HTPB Propellants Subjected to Abnormal Environments*

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Determining the optimum and safe operational logistics for motors filled with AP/Al/HTPB propellants, performing probability risk assessment associated with accident scenarios, and the future design of high performance low vulnerability propellants all share a common requirement: the ability to predict the hazards response and violence from the propellant, as a function of the material parameters in the propellant formulation, when the system is subjected to abnormal environments. In this paper, we discuss the development of an integrated chemical-thermal-mechanical-hydrocode for predicting the response of AP/Al/HTPB based propellants in scenarios involving thermal, impact, and shock stimuli. The integrated hydrocode is based on the ALE3D computational platform incorporated with models describing 1) the mechanical response of the propellant when subjected to impact and shock loading, 2) the thermal transport associated with external thermal sensitization and internal energy release from chemical reactions, 3) the reaction kinetics of AP/HTPB and subsequently the products with aluminum, and 4) ignition criterion, combustion mechanism, and the transition to a rapid and violent event. The models within the ALE3D structure are linked dynamically with each other so that we can account for feedback effects; the mechanical response of the system to both an external and internal thermal stress from a fire and chemical reaction in the propellant, respectively, the latter initiated by the external thermal stress. To validate the model parameters, a series of AP/Al/HTPB compositions, 90wt% solids loaded, were formulated and subjected to various experiments involving impact, thermal sensitization, and shock loading. Material parameters, such as AP and Al particle size, wt% of combustion modifiers, and binder mechanical properties were varied systematically in the formulations in order to study their effects on the reaction kinetics, ignition threshold, and combustion mechanism. The incorporation of material parameters in the models allow us to optimize the tradeoff between performance and vulnerability of future propellant formulations.

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